

1-Chloro-1-nitropropane
600-25-9 | DTXSID2024797

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.78 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.24e-01

Confidence level: 7.98e-01

Nearest Neighbors from the Training Set

Image not found

Propane, 2-methyl-2-nitro-

Measured: 16.9

Predicted: 9.73

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Ethyl 2-bromoisobutyrate

Measured: 7.79

Predicted: 3.11

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Ethyl methyl sulfide

Measured: 6.88

Predicted: 121

Image not found

Ether, isobutyl methyl

Measured: 3.79

Predicted: 201

Image not found

2,3,3-Trimethyl-1-pentene

Measured: 3.10

Predicted: 35.2